

Three-Dimensional Computational Fluid Dynamics Simulations of Local Particle Deposition Patterns in Lung Airways

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Introduction

■ EPA has identified respirable particulate matter (PM) as a significant threat to human health, particularly in the elderly, in children, and in persons with respiratory disease.

■ Deposition of PM in the respiratory system is highly variable, depending upon particle characteristics, airway dimensions, and ventilatory conditions.

■ This complexity complicates the study of the health risks associated with inhaled PM.

■ Computational predictions of PM can be made at many different spatial resolutions (Figure 1).

■ In the present study, 3D Computational Fluid Dynamics (CFD) models of generational and localized PM deposition were validated using data from published experimental studies of PM deposition in human lung casts.

■ The ability of CFD to appropriately simulate trends in deposition patterns due to changing ventilatory conditions was specifically addressed.

Methods

■ CFD was used to model the experimental hollow cast system (Figure 2) of Schlesinger et al. (*Ann. Occup. Hyg.* 1-4:47-64, 1982).

■ A digital 3D model of the trachea and main bronchi of the experimental human cast (Figure 3A) was created from reported cast morphometric data using GAMBIT modeling software (Fluent, Inc., Lebanon, NH).

■ CFD simulations of airflow were performed in the modeled system using Fluent Inc.'s FIDAP CFD software.

■ A set of 1000 particles was entrained in the inlet airflow using FIDAP's two-phase model. Particles 8 μ m in diameter were considered for constant input flow rates of both 15 and 60 L/min.

■ Both plug and parabolic input flow profiles were considered (Figure 3B).

■ A numerical, deterministic model (AERODEP, Figure 4) was also used to predict overall tracheal deposition.

■ The overall deposition values and simulated spatial patterns within the bifurcation were compared with the reported experimental results.

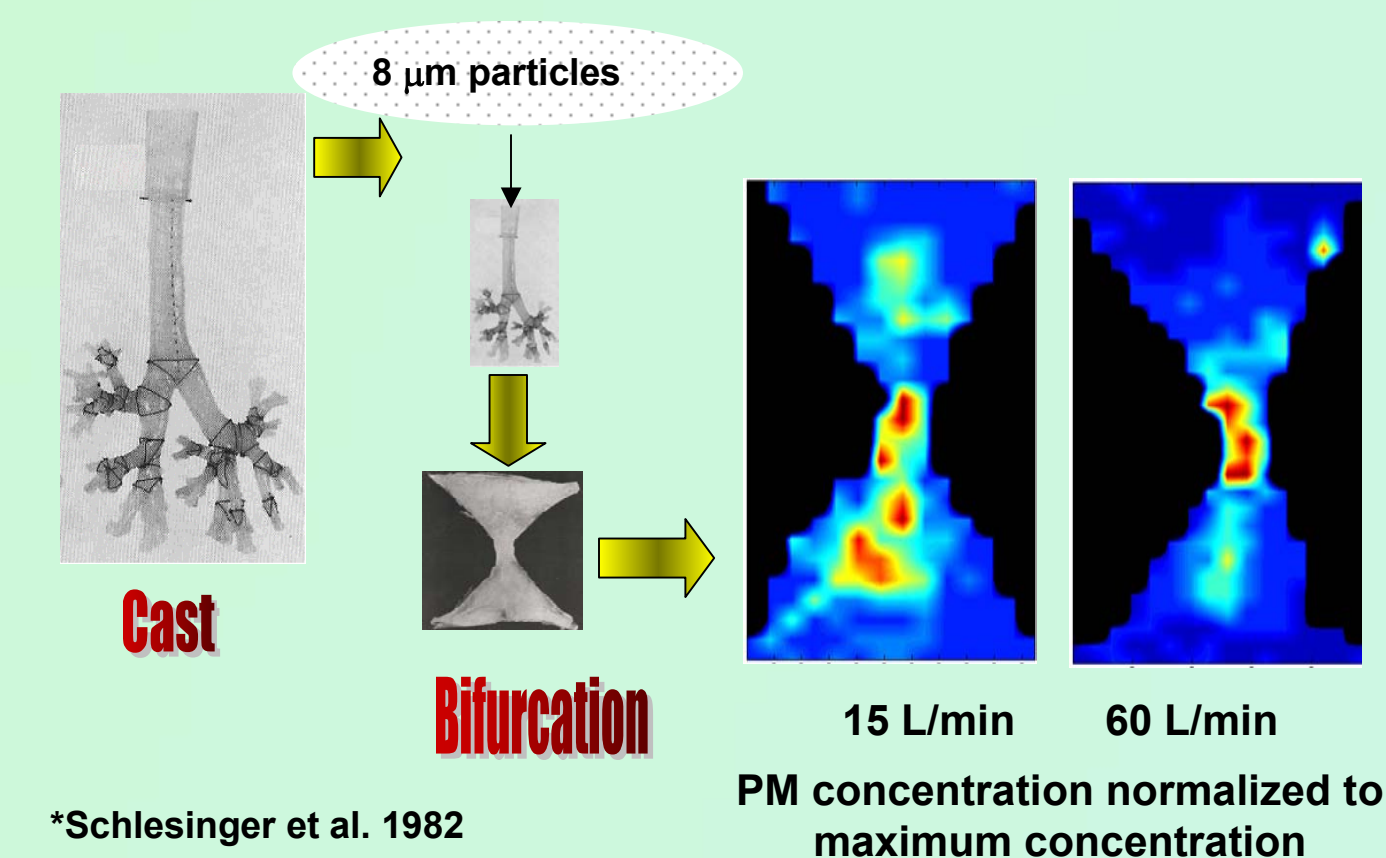


Figure 2. Microdosimetry Measurements of PM Deposition in a Cast of the Human Tracheobronchial Region. Particles (ferric oxide, 8 μ m in diameter) were introduced into a silicon replica cast of the human upper tracheobronchial region. After exposure, the bifurcation region of the trachea was cut open and the deposition of particles was determined by microscopic examination.

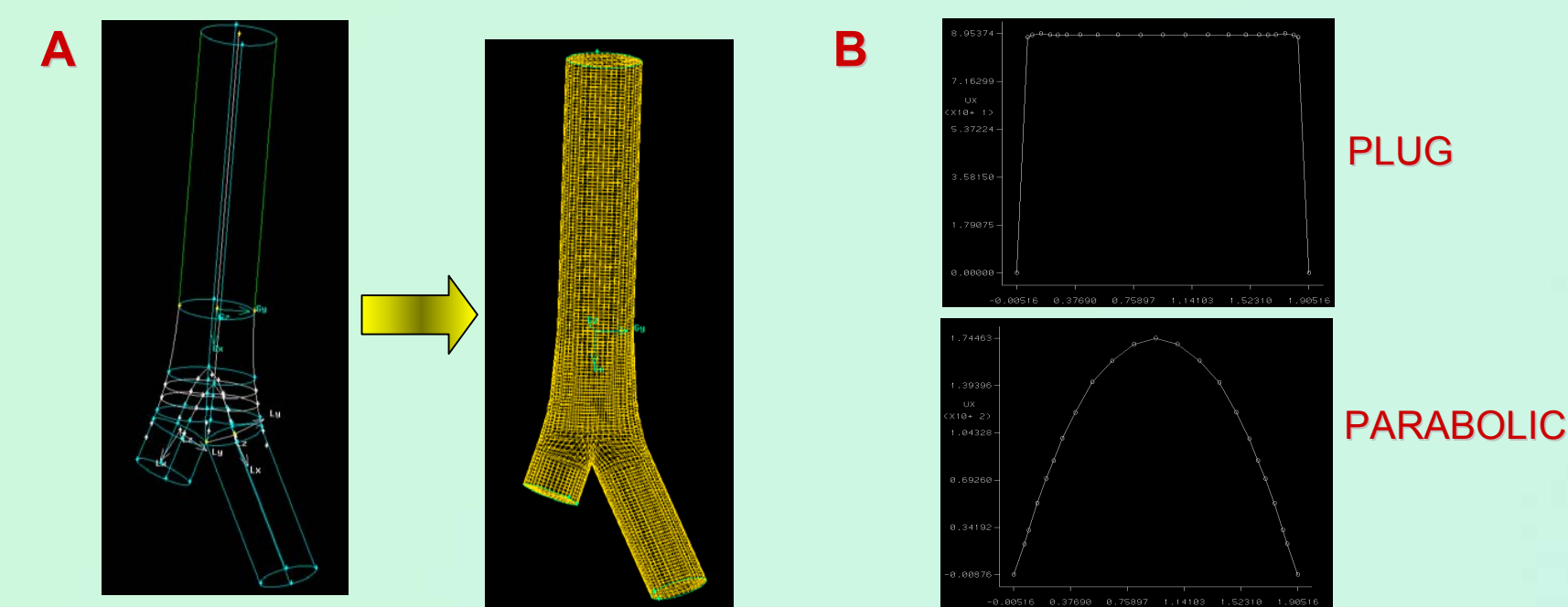


Figure 3. CFD Model Geometry and Inlet Velocity Profiles. A) The geometry was created from the published morphometric data and the three-dimensional spatial mesh for the solution of the fluid flow and particle motion was constructed. B) Example input velocity profiles.

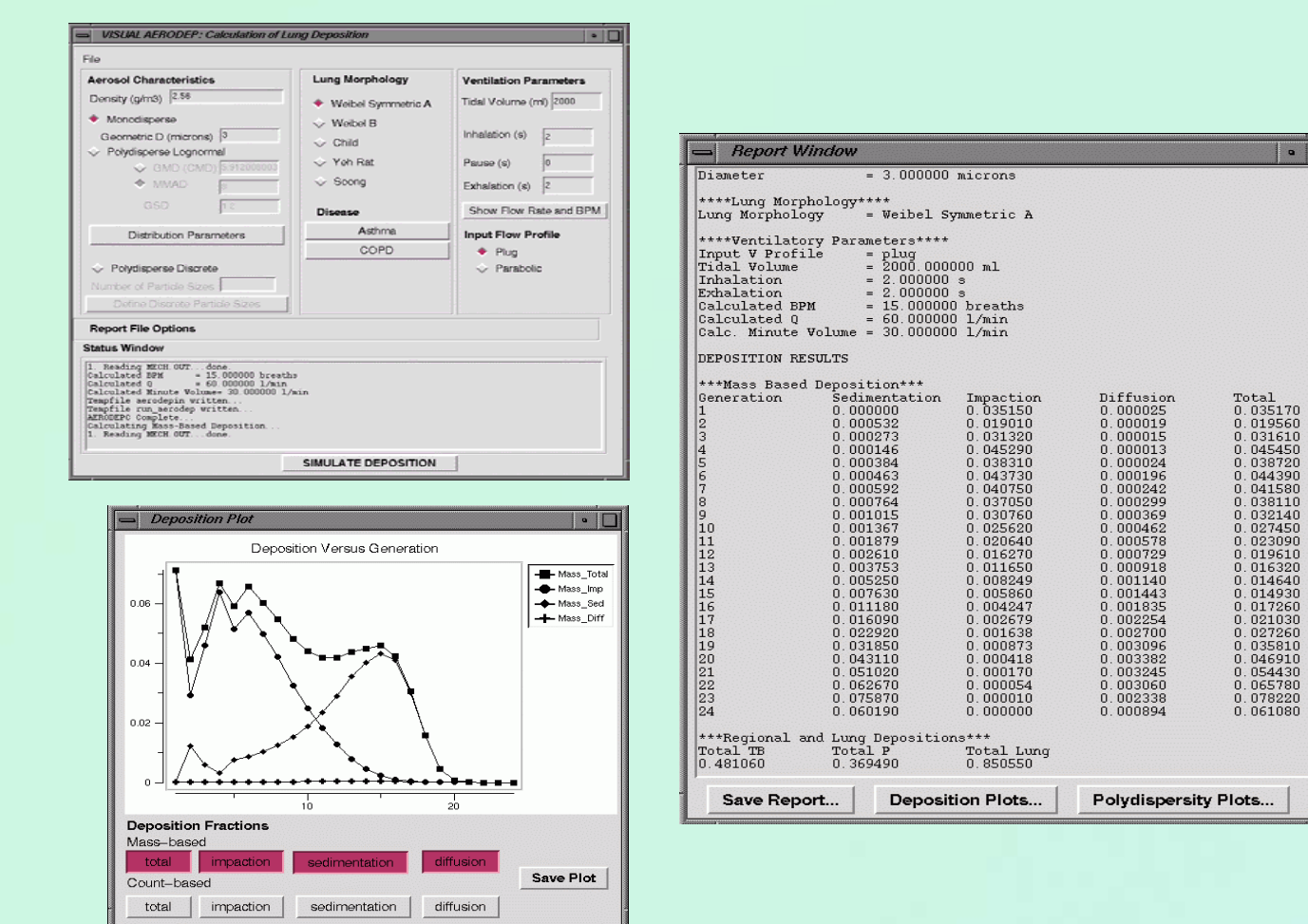


Figure 4. AREODEP Environment for Deposition Simulations. AREODEP, an interactive environment for the prediction of regional and generational lung PM deposition, was used to simulate tracheal deposition of 8 μ m particles for the experimental flow conditions considered.

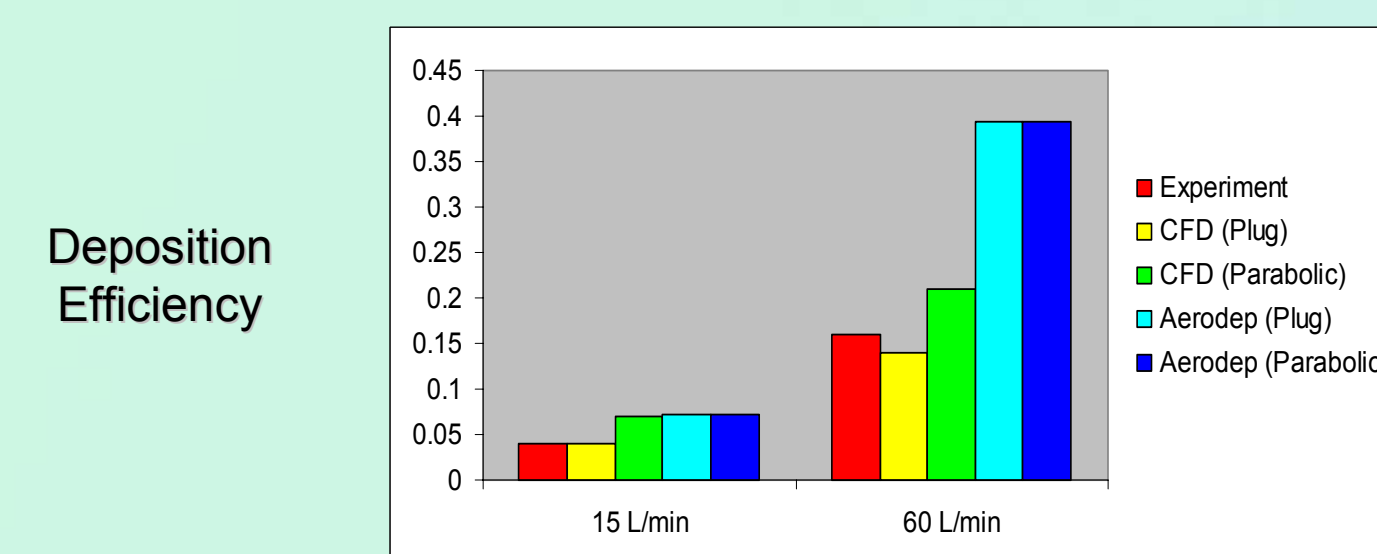


Figure 5. PM Deposition in the Tracheal Bifurcation. The deposition efficiency (number of particles deposited/number of particles inhaled) as predicted by both AERODEP and CFD for various combinations of flow rate and inlet velocity profile.

Results

■ Deposition efficiencies in the trachea as determined by CFD and AERODEP simulations are given in Figure 5. In general, the CFD simulations provided a better estimate of tracheal deposition than the AERODEP simulations.

■ Airflow (velocity vectors, Figure 6A) and example particle paths (8 μ m particles, Figure 6B) are presented below for laminar flow conditions for flows of 15 and 60 L/min. Results for both plug and parabolic profiles are given.

■ The CFD simulations predicted non-uniform deposition patterns (Figure 7) similar to those seen in the experimental system. Deposition in the bifurcation of the trachea was greater for inlet parabolic velocity profiles. A better model considering local surface features and a more completely characterized input velocity profile may be necessary to exactly reproduce the experimental patterns.

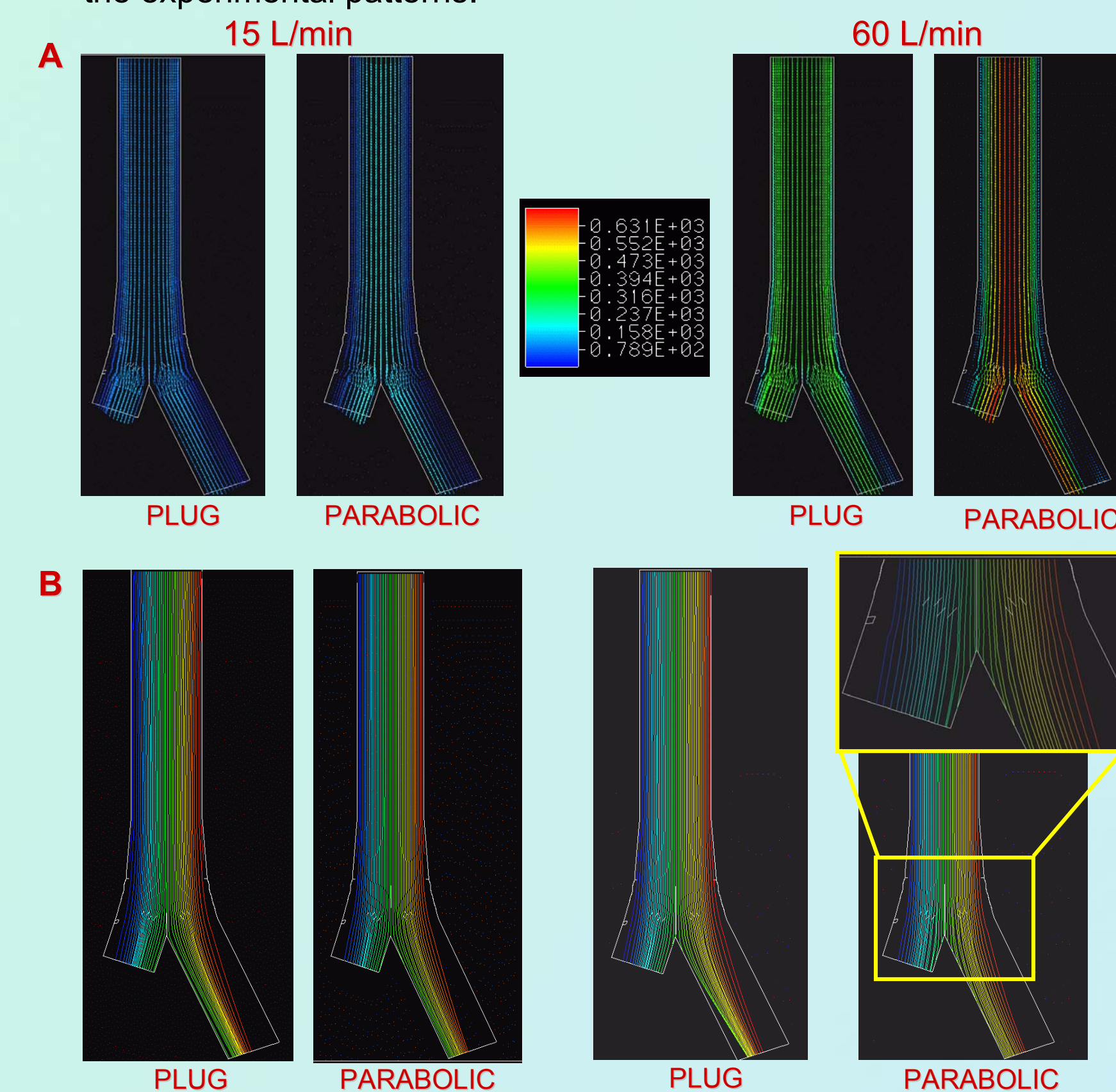


Figure 6. Airflow Patterns and Particle Paths. A) The magnitude of flow velocity is given by the color of the vectors. B) Paths for 40 particles. Note the impact of the particles in the bifurcation in the expanded view.

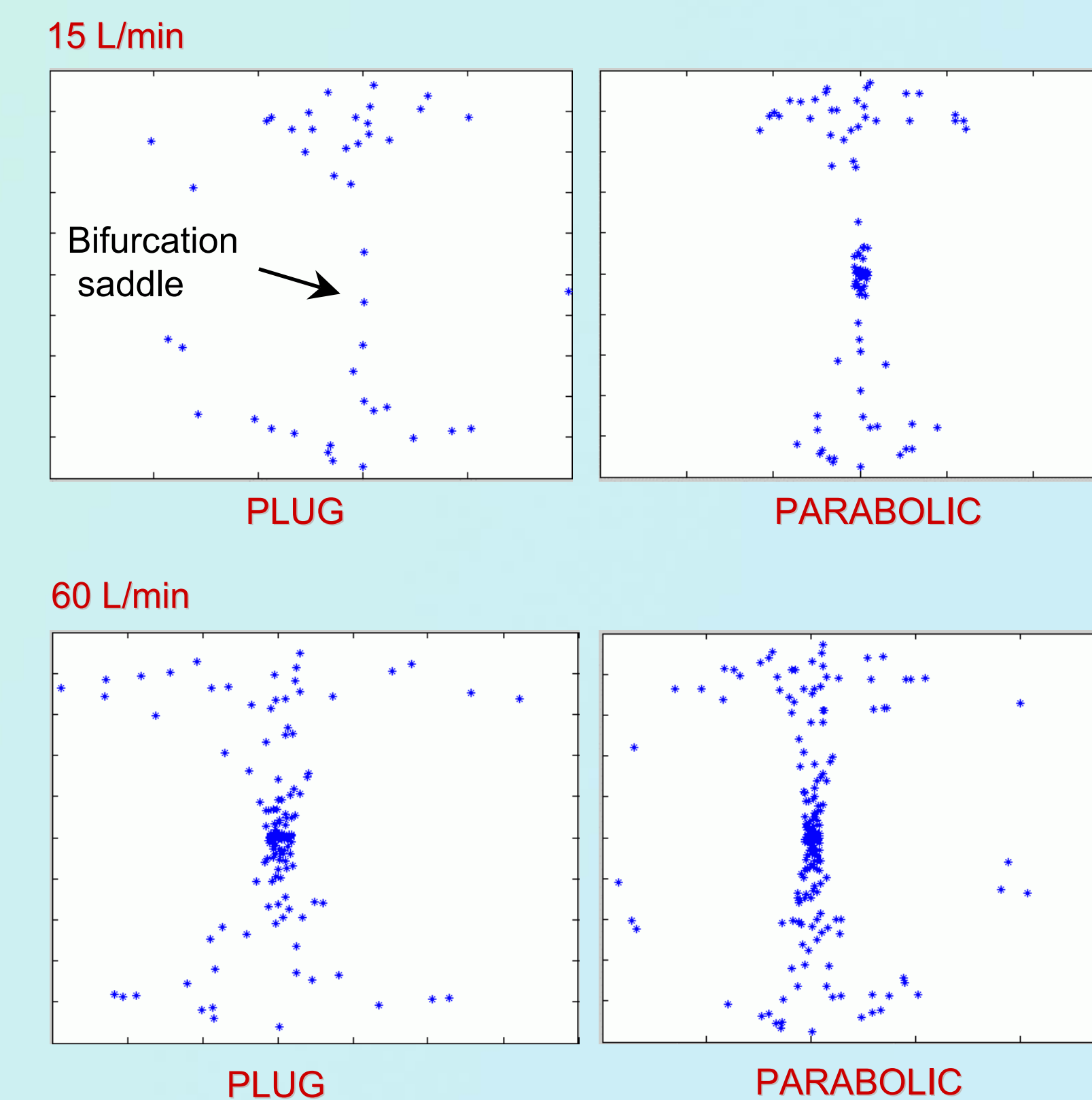


Figure 7. CFD Simulations of Deposition Patterns in the Bifurcation Region. Note the increased concentration of particles in the bifurcation saddle (as compared to other regions) at 60 L/min, as seen in the experimental system.

Conclusions and Impact

■ The CFD models provided better prediction of total tracheal deposition efficiency than did the simplified numerical models.

■ PM deposition proved to be particularly sensitive to input flow conditions.

■ The local deposition patterns predicted with the CFD models were consistent with experimentally-obtained patterns.

■ CFD models may provide an efficient means of studying the complex influence of airway geometry, particle characteristics, and ventilatory parameters on PM deposition in the lungs.

Future Directions

■ Valid 3D CFD models will be invaluable tools in predictive studies of PM deposition, as the effects of a wide range of particle characteristics, lung physiologies, and ventilatory conditions can be rapidly studied.

■ The influence of turbulent and cyclic air flows and local airway features such as cartilaginous rings and carinal ridges will also be studied.